Solution 5

Exercise 1: The space charge is given by $Q_{sc} \approx qN_D W_D$. N_D is the donor concentration and W_D is the depletion width. We begin to solve Poisson's equation in order to have an expression for W_D as a function of ψ_{bi} that is the built-in potential in the semiconductor, defined as (see figure 1):

$$\psi_{\text{bi}} = \phi_n(0) - \phi_n(W_D) \tag{1}$$

We use the approximation of abrupt junction: $\rho \approx qN_D$ for $x < W_D$ and $\rho \approx 0$ $(E = 0)$ for $x > W_D$ to solve Poisson's equation:

$$\frac{d^2\phi(x)}{dx^2} = -\frac{dE(x)}{dx} = \frac{\rho(x)}{\epsilon_s} \tag{2}$$

By integrating it one time, we get:

$$E(x) = -\frac{\rho(x)x}{\epsilon_s} + c_1 \tag{3}$$

$$E(x) = -\frac{qN_D x}{\epsilon_s} + c_1 \text{ for x} < W_D \tag{4}$$

$$\tag{5}$$

Because the electric field has to be continuous at $x = W_D$ we have:

$$E(W_D) = 0 = -\frac{qN_D W_D}{\epsilon_s} + c_1 \tag{6}$$

$$c_1 = \frac{qN_D W_D}{\epsilon_s} \tag{7}$$

$$E(x) = -\frac{qN_D(W_D - x)}{\epsilon_s} \text{ for x} < W_D \tag{8}$$

By integrating a second time we get:

$$\phi(x) = \frac{qN_D W_D x}{\epsilon_s} - \frac{qN_D x^2}{2\epsilon_s} + c_2 \text{ for x} < W_D \tag{9}$$

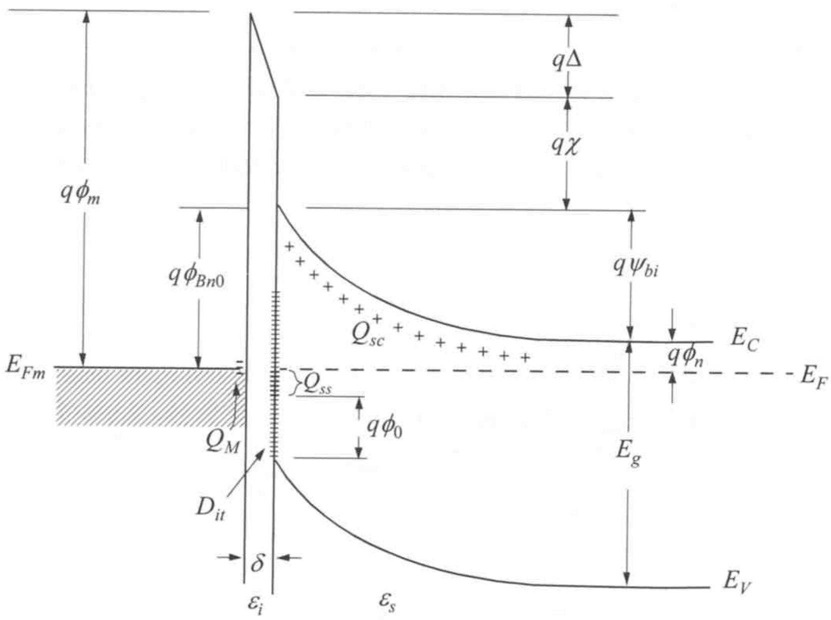
$c_2 = 0$ because $\phi(0) = 0$ for the abrupt junction approximation. Using (1) we get:

$$\psi_{\text{bi}} = \phi(0) - \phi(W_D) = \frac{qN_D W_D^2}{2\epsilon_s} \tag{10}$$

$$W_D = \sqrt{\frac{2\epsilon_s \psi_{\text{bi}}}{qN_D}} \tag{11}$$

And finally:

$$Q_{sc} \approx qN_D W_D = \sqrt{2\epsilon_s \psi_{\text{bi}} qN_D} = \sqrt{2\epsilon_s qN_D(\phi_{\text{Bn0}} - \phi_{\text{n}})} \tag{12}$$



ϕ_m = Work function of metal
ϕ_{Bn0} = Barrier height (without image-force lowering)
ϕ_0 = Neutral level (above E_V) of interface states
Δ = Potential across interfacial layer
χ = Electron affinity of semiconductor
ψ_{bi} = Built-in potential
δ = Thickness of interfacial layer
Q_{sc} = Space-charge density in semiconductor
Q_{ss} = Interface-trap charge
Q_M = Surface-charge density on metal
D_{it} = Interface-trap density
ε_i = Permittivity of interfacial layer (vacuum)
ε_s = Permittivity of semiconductor

Detailed energy-band diagram of a metal-*n*-semiconductor contact with an interfacial layer (vacuum) of the order of atomic distance. (After Ref. 14.)

Figure 1: Schottky junction with interfacial layer.

By looking carefully on figure 1 we obtain for the interface-trap charge density:

$$Q_{ss} = -qD_{it}(E_g - q\phi_0 - q\phi_{Bn0}) \tag{13}$$

The quantity in parentheses is the energy difference between the Fermi level at the surface and the neutral level of interface states above E_V (ϕ_0). The interface-trap density D_{it} times Q_{ss} yields the number of surface states above the neutral level that are full.

Δ is obtained by again looking on the band diagram figure 1:

$$\Delta = \phi_m - (\chi + \phi_{Bn0}) \tag{14}$$

This relation results from the fact the Fermi level must be constant throughout this system at thermal equilibrium.

By combining equation (14), (12), (13), $\Delta = -(\delta Q_m/\epsilon_i)$, $\psi_{\text{bi}} = \phi_{Bn0} - \phi_n$ and $Q_M = -(Q_{sc} + Q_{ss})$ we obtain:

$$\phi_m - (\chi + \phi_{Bn0}) = \sqrt{\frac{2\epsilon_s q N_D \delta^2}{\epsilon_i^2}(\phi_{Bn0} - \phi_n)} - \frac{q D_{it} \delta}{\epsilon_i}(E_g - q\phi_0 - q\phi_{Bn0}) \tag{15}$$

If we replace some constants with:

$$c_1 = \frac{2q\epsilon_s N_D \delta^2}{\epsilon_i^2} \tag{16}$$

and

$$c_2 = -\frac{\epsilon_i}{\epsilon_i + q^2 \delta D_{it}} \tag{17}$$

we obtain:

$$\phi_m - (\chi + \phi_{Bn0}) = \sqrt{c_1(\phi_{Bn0} - \phi_n)} - \frac{c_2 + 1}{q}(E_g - q\phi_0 - q\phi_{Bn0}) \tag{18}$$

This equation can be rearrenged to express ϕ_{Bn0} as a function of ϕ_m. We let this last calculation to the math lovers.

In the case of a-Si:H, Wronski and Carlson got a linear relation between ϕ_{Bn0} and ϕ_m. As one can observe on the graph, the workfunctions of the studied metals very from 4 to 5.5 eV, but the induced barrier heights vary only from 0.7 to 1 eV. Thus, we conclude that Q_{sc} and Q_{ss} attenuate significantly the effect of ϕ_m.